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EFFECT OF MOLECULES AND GRAINS ON ROSSELAND MEAN OPACITIES

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ABSTRACT

Rosseland mean opacities, which include the effects of molecules and grains, have been computed down to 630 K. Molecular effects have been computed with the opacity sampling method wherever possible. A detailed treatment of the condensation of and absorption due to grains has also been included for magnesium silicates and iron. The contributions of molecules (between 3000 K and 1500 K) and grains (below 1600 K) are several orders of magnitude above the Rosseland mean opacity computed without them. The overall metal abundance and the C/O ratio can also dramatically affect the total opacity.

Subject headings: molecular processes — opacities

I. INTRODUCTION

Whenever the structure of an astrophysical plasma is computed using the diffusion approximation for the radiative transfer equation, the Rosseland mean opacity is required as an input quantity. Most investigators use the standard compilation of Cox and Stewart (1970*a*, *b*) or the more recently available Los Alamos opacity library program. However, for temperatures below 4000 K, bound-bound transitions in molecules, which are not included in the Cox-Stewart calculations, become important. At temperatures below about 1500 K, scattering and absorption from solid grains also become important. These temperatures occur in the envelopes of stars with effective temperatures less than about 5000 K and during the collapse of protostellar and planetary clouds.

A number of calculations have included some low-temperature absorbers. Gaustad (1963) included the effects of ice, silicate grains, and some molecules for use in his investigations of star formation. Gilra (1972) and Jones and Merrill (1976) also included the effects of silicate grain opacity in their studies of circumstellar shells. Auman and Bodenheimer (1967) included the effect of water vapor for temperatures between 1680 K and 4200 K, based upon Auman's (1966) harmonic mean opacities. Tsuji (1971) included the effects of seven different molecules, including water and titanium oxide, in a calculation based upon the Elsässer band model. Cameron and Pine (1973) improved the treatment of grains by utilizing more complete optical constants for both silicates and iron grains. Alexander (1975) made the first attempt to compute reasonably complete and detailed low-temperature opacities. That study used straight mean opacities of four molecules, band-averaged opacities for 13 other molecules, and an approximate treatment of silicate grains to present Rosseland opacities for a variety of compositions at temperatures from 700 K to 10,000 K.

Table 1 illustrates the divergence of results over the years. As more detailed molecular and solid absorbers have been included, the mean opacity has become progressively larger. Alexander's (1975) results probably represent an upper limit for the molecular sources because of his use of straight mean opacities.

Two recent advances allow for improvement over previous calculations of low-temperature Rosseland mean opacities. The development of the opacity sampling method (Peytreman 1974; Sneden, Johnson, and Krupp 1976) allows detailed information concerning millions of atomic and molecular lines to be utilized in the calculation of opacities, so that no averaging or smearing is necessary. The laboratory study of the optical constants of magnesium silicates by Day (1979) provides a corresponding increase in the precision possible in computing the opacity due to grains. Both of these improvements have been included in the present investigation.

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TABLE 1

OPACITY COMPARISON (log κ at log $\rho = -10.$)

SOURCE	TEMPERATURE (K) 3000	2000	1000
Tsuji 1966	−4.2	−5.4	−8.5
Auman and Bodenheimer 1967	−3.1	−2.9	...
Cox and Stewart 1970*a*, *b*	−4.2	−4.7	...
Tsuji 1971	−3.3	−3.8	...
Cameron and Pine 1973	−4.8	−5.9	−0.4
Alexander 1975	−3.9	−1.8	0.0
Present study	−4.0	−2.8	+0.1

The Rosseland mean opacity for a solar composition is presented in tabular form for use in structure calculations. An analysis of the significance of different absorbers as a function of temperature is presented. The effects of lowering the metal abundance and changing the carbon abundance (to simulate an S star or carbon star) are also examined.

II. PROCEDURE

The Rosseland mean opacity is the appropriate opacity to use with the diffusion approximation of the radiative transfer equation and is often used in other approximate ways as well. Specifically, it is defined as:

$$\frac{1}{\kappa_R} = \frac{\int_0^\infty (1/\kappa_\nu)(\partial B_\nu/\partial T)\, d\nu}{\int_0^\infty (\partial B_\nu/\partial T)\, d\nu}. \qquad (1)$$

Clearly the important difficulty in the above equation is in the calculations of κ_ν since, for any particular temperature and pressure, the rest of the factors in equation (1) are known. We discuss the opacities used in this paper under three headings: continuous opacities, line opacities, and grain opacities.

a) *Continuous Opacities*

Continuous opacities are those in the ATLAS5 code which have been well discussed in the literature (Kurucz 1970) and used in many atmospheric calculations. For this calculation we specifically include bound-free and free-free absorption due to H I, He I, Mg I, C I, Al I, Si I, N I, O I, Mg II, Si II, and Ca II. Rayleigh scattering due to H I, H_2, and He I are accounted for. Finally, the opacity due to H^- and the other ions He^-, H_2^-, and H_2^+ are accounted for.

b) *Line Opacities*

A major improvement over previous work is the calculation of bound-bound opacities by the opacity sampling (OS) technique, as described by Peytremann (1974) and Sneden, Johnson, and Krupp (1976). In the OS method, the opacities at each selected frequency are treated as accurately as possible by summing the absorption coefficients due to all the atomic and molecular lines and continuous sources which contribute there. Here we use 1,010 frequencies—the set used by Johnson, Bernat, and Krupp (1980), which has been shown to be easily adequate for the integrated fluxes of model atmospheres of cool giant stars (Peytremann 1974; Johnson and Krupp 1976).

Bound-bound transitions include 35,000 atomic lines (line list kindly provided by R. Bell and augmented by 3000 UV Fe I lines from R. Kurucz) and hundreds of thousands of lines of the following molecules: CN (violet and red systems), CO (infrared vibration-rotation bands), C_2 (Swan, Phillips, and Ballik-Ramsay systems), TiO (α, γ, γ', δ, and ϕ systems), CH (G band), NH ($A\ ^3\pi$-$X\ ^3\Sigma$ system), MgH ($A\ ^2\pi$-$^2\Sigma$ system), and OH ($A\ ^2\Sigma'$-$X\ ^2\Sigma$ system). In addition, we use 100 cm^{-1} straight mean opacities to represent H_2O.

In the line absorption coefficient we assume a nonthermal broadening or microturbulence of 1 km s^{-1}. For atomic lines, a Voigt profile is used with a damping coefficient equal to the sum of the Van der Waals (Unsold 1955) and 3 times the classical radiation value. Molecular lines are assumed to have pure Doppler broadening. We adopt the molecular and atomic data from the work of Johnson, Bernat, and Krupp (1980) with the correction to C_2 from Johnson (1982), and the reader is referred to those papers for additional data, comments, and sources.

c) *Grain Opacities*

The computation of accurate grain opacities depends upon a knowledge of three quantities: the amount and chemical composition of the material which has condensed out of the gaseous phase, the distribution of grain sizes, and the optical properties of the grains.

The amount of condensed material can, in principle, be determined from a detailed application of the law of mass action to all the major solid and gaseous compounds which may be present. Such a calculation has been performed by Grossman (1972), who considered 75 gaseous species of 20 elements and 92 solid condensates. He presented results for the silicates and for iron as percentages of each element in the solid phase as a function of temperature.

We use these curves, scaled as a function of pressure according to the relation given by Grossman (1972) for the condensation temperature, to determine the amount of magnesium, silicon, oxygen, and iron in the condensed forms of enstatite ($MgSiO_3$), forsterite (Mg_2SiO_4), and metallic iron at each required temperature and pressure. The amount of each of these elements in the condensed form is then subtracted from the actual abundance of the element for purposes of computing the gaseous equilibrium. The effects of the presence of silicates of less abundant elements, such as calcium and aluminum, are treated approximately, even though they never account for more than 15% of the condensed silicates because some of them condense at higher temperatures than the magnesium silicates. Their contribution to grain formation is included with that of forsterite.

Ionization and dissociation are handled by ATLAS5, with the alterations made by Johnson, Bernat, and Krupp (1980) for treating the opacities of trace elements. Grains of carbon-containing materials are not considered here because calculations for temperatures at which solid condensates can form were only carried out for oxygen-rich compositions.

In a condensing gas, the solid condensates will form grains or "dust." Although the theory of grain formation is beyond the scope of this investigation, the physical characteristics, such as shape, size, and number of the grains, are all important to the opacity calculation.

From studies of interstellar polarization and of dust samples from space and Earth, grains are found to have a number of shapes: oblate and prolate spheroids, needles, plates, and spheres. To perform opacity calculations considering all these shapes would be impractical since neither theoretical results nor empirical data exist for the relative distribution of grain shapes or for the interaction of light with many of the possible shapes. For these reasons, all grains are assumed to be spherical in shape.

The distribution of grain sizes also represents a difficult theoretical and observational problem. Observations of interstellar extinction indicate that the grain size is on the order of a few tenths of a micrometer (μm). Mathis, Rumple, and Nordsieck (1977) obtain a best fit to observations with a power-law size distribution,

$$n(a) = ka^{-3.5}, \qquad (2)$$

where a is the grain radius in micrometers. It is unfortunately not known whether this relationship applies to grains within stellar atmospheres or circumstellar shells. Almost certainly, the history of the condensing medium will affect many grain characteristics, including average grain size, grain shape, and grain composition and purity. For example, some observations indicate that interstellar grains may be "dirty" combinations of several materials. Little information is presently available to justify extending these calculations to include these complications. Test calculations with optical parameters determined from terrestrial and lunar samples indicate that the final Rosseland mean opacity would probably differ from the present results by a factor of no more than 3.

The average grain size of silicate grains was taken to be 0.11 μm. Several investigators (Huffman and Stapp 1971; Wickramasinghe and Nandy 1971) have suggested that iron grains are considerably smaller than the silicate grains. Following the conclusion of Wickramasinghe and Nandy, an average iron grain size of 0.02 μm has been used. After the total amount of a particular condensate has been determined from Grossman's (1972) condensation curves, the constant k in equation (2) is determined by the condition

$$\rho_{gr} = \rho_g \sum_a n(a) 4/3\pi a^3 ,$$

where ρ_{gr} is the density of grains suspended in each cubic centimeter of the medium and ρ_g is the density of material within a grain. The density of grain material is set at 3 g cm^{-3}.

The extinction due to grains was computed according to the Mie theory (see, e.g., Wickramasinghe 1973) for spherical particles as a function of grain radius (a). The input quantity required for this calculation is the complex index of refraction as a function of wavelength. The most complete indices of refraction for enstatite and forsterite are provided by Day (1979). He measured the optical properties of particles condensed from the vapor over a wavelength range from 7 μm to 33 μm. Unfortunately, these data require extrapolation to cover the full wavelength region of interest. Pollack, Toon, and Khare (1973) obtained the index of refraction for five naturally occurring terrestrial rocks over the wavelength range from 0.2 μm to 50 μm. Figure 1 illustrates the effect on the Rosseland mean opacity of using these different indices of refraction. The divergence among

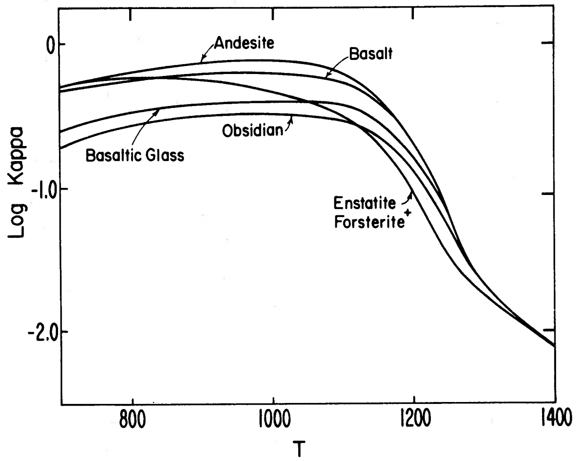

FIG. 1.—The Rosseland mean opacity is plotted as a function of temperature, at fixed $P_g = 0.1$ dynes cm^{-2}, for several choices of grain optical parameters. The curve labeled "enstatite and forsterite" was computed using the indices of refraction of Day (1979). The other four curves used indices of refraction found by Pollack, Toon, and Khare (1973) for terrestrial rocks.

TABLE 2

MASTER GRID FOR ROSSELAND MEAN OPACITIES (log κ)

	LOG ρ																
LOG T	−18.	−17.	−16.	−15.	−14.	−13.	−12.	−11.	−10.	−9.	−8.	−7.	−6.	−5.	−4.	−3.	−2.
4.00									0.864	1.468	1.799	2.026	2.270	2.578	3.008	3.537	4.016
3.90								−0.133	0.033	0.194	0.426	0.746	1.126	1.574	2.101	2.510	
3.80								−1.436	−1.474	−1.226	−0.832	−0.362	0.181	0.782	1.339	1.780	
3.70								−2.919	−2.843	−2.420	−1.769	−0.988	−0.243	0.341	0.817	1.261	
3.65								−3.557	−3.317	−2.654	−1.854	−1.114	−0.492	−0.002	0.459	0.913	
3.60							−3.917	−3.812	−3.355	−2.703	−2.035	−1.415	−0.838	−0.343	0.065		
3.55							−4.015	−3.816	−3.474	−2.996	−2.389	−1.657	−1.025	−0.613	−0.290		
3.50							−4.090	−4.065	−3.888	−3.358	−2.410	−1.530	−1.122	−0.908	−0.585		
3.45						−4.296	−4.436	−4.492	−4.076	−2.986	−1.957	−1.495	−1.343	−1.227			
3.40						−4.770	−4.850	−4.410	−3.289	−2.208	−1.729	−1.619	−1.573	−1.509			
3.35						−5.095	−4.537	−3.341	−2.404	−1.976	−1.821	−1.764	−1.734	−1.709			
3.30					−5.130	−4.442	−3.584	−3.150	−2.771	−2.411	−2.093	−1.919	−1.858	−1.828			
3.25				−5.052	−4.214	−3.875	−3.979	−4.002	−3.696	−3.140	−2.595	−2.207					
3.20				−4.085	−4.215	−4.558	−4.873	−4.893	−4.483	−3.906	−1.558						
3.15			−4.383	−4.744	−5.122	−5.401	−5.602	−1.845	−3.174	−1.411	−0.169						
3.10			−5.372	−5.600	−1.942	−5.055	−1.656	−1.373	−0.401	0.130							
3.05			−6.142	−2.783	−1.427	−1.293	−0.393	0.050	0.154	0.201							
3.00		−1.471	−1.418	−0.882	−0.310	0.008	0.097	0.133	0.138								
2.95		−0.716	−0.187	−0.012	0.038	0.076	0.097	0.100	0.100								
2.90	−0.109	−0.034	0.018	0.048	0.058	0.057	0.063	0.063									
2.85	−0.001	0.018	0.027	0.030	0.032	0.032	0.032	0.032									
2.80	0.001	0.005	0.006	0.006	0.006	0.006	0.006										

the results is well within that required by other approximations contained in these calculations. Because the data of Day match the chemical form of the condensates of interest, his data have been adopted here.

A similar situation exists for the indices of refraction of metallic iron. Leksina and Penkina (1967) published data for the wavelength range from 0.4 μm to 5 μm. Once again, various extrapolations produced relatively small variations in the overall Rosseland mean opacities. The total opacity including iron is approximately 0.5 dex greater than the total opacity excluding iron.

III. RESULTS

Rosseland mean opacities are computed at a range of pressures for the temperature range from 10,000 K to 700 K. Tables in temperature and density are produced by bi-cubic spline interpolation with a program provided by VandenBerg (1980). The standard chemical composition is that of Cameron (1968), as modified by Cameron and Pine (1973). Results for this composition are presented in Table 2 as mass absorption coefficients (cm^2 g^{-1}). The higher temperature results are given only for the purpose of convenient fitting to the standard Los Alamos opacities. No detailed attempt has been made to incorporate all the high-temperature absorbers. Molecular effects disappear from the Rosseland mean opacity before temperatures of 6000 K are reached.

Figure 2 compares these results with the earlier computations of Alexander (1975). The most pronounced differences occur in the temperature region where grain condensation occurs. Alexander's crude treatment of grains assumed immediate condensation of all silicates as soon as the condensation temperature of the first silicate (Al_2SiO_5) was reached. The resulting rise to high opacity values thus occurs too quickly and at too high a temperature. The present results show a pronounced opacity minimum between 1400 K and 1800 K at all densities.

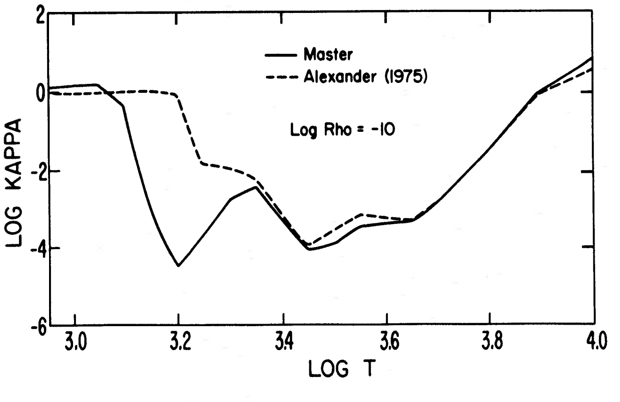

FIG. 2.—The results of the present study are compared with the results presented by Alexander (1975) at a density of 10^{-10} g cm^{-3}. The major discrepancy that occurs at 1600 K results from Alexander's assumption of complete silicate condensation at the condensation temperature of the first silicate. The present results show both a cooler and a more gradual opacity rise due to grains.

The opacity due to grains also differs from the results reported by Cameron and Pine (1973) and by Pollack (DeCampli and Cameron 1979). The rise to the opacity plateau is more gradual for the present results, usually spanning 200 K or more range in temperature. The results both of Cameron and Pine and of Pollack show discontinuities in the total opacities at grain condensation, contrary to the results of Grossman (1972). Otherwise, our results are intermediate between those of Cameron and Pine, who report cooler condensation temperatures and lower grain opacities, and those of Pollack, who reports higher condensation temperatures and larger grain opacities.

Modest differences with Alexander's (1975) earlier work are also seen at the somewhat higher temperatures where molecular absorbers are important. The use of opacity-sampled molecular opacities for all molecules except water vapor generally diminishes the Rosseland mean opacity. This is to be expected because the straight mean opacities used by Alexander underemphasize the effect of gaps between the molecular lines. The inclusion of a straight mean approximation to the opacity of water vapor in the present results will produce an overestimate of the total opacity for all temperatures from 3200 K, where water vapor first becomes an important absorber, down to the temperature at which grains begin to condense, about 1300 K. This effect occurs at all densities but is greatest at higher densities. This temperature range extends to lower temperatures than predicted by the earlier work by Alexander because of the cooler onset of grain condensation in the present work. Although it is difficult to estimate the magnitude of the uncertainty introduced by this approximation, it would be very desirable to have available sufficient data to include water vapor in the opacity-sampled calculation.

The relative effects of molecules and grains on the total opacity are illustrated in Figure 3. Because the Rosseland mean is a harmonic mean, the opacity due to different absorbers cannot be calculated separately to be added together later. In this calculation the Rosseland mean absorption coefficient is simultaneously calculated for all sources and for various combinations of all sources except one. Thus, for example, the curve identified as "no molecules" is the Rosseland mean opacity of all sources *except* molecules.

Once again, the overwhelming influence of grains is seen at the lower temperatures. If solid condensates are ignored, errors of several orders of magnitude can occur. At somewhat higher temperatures, molecules can also be very important; at some densities, for example, the neglect of molecules can give rise to errors of three orders of magnitude. These effects are likely to be of extreme importance in computing the structure of the

1983ApJ...272..773A

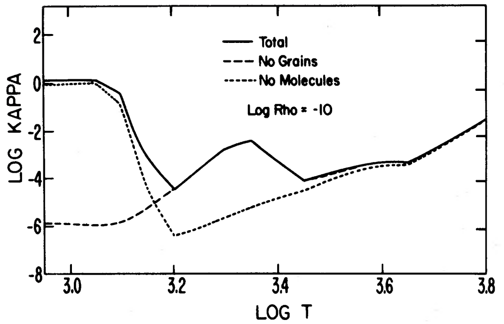

FIG. 3.—The Rosseland mean opacity computed with different sources turned off is compared with the total opacity at a density of 10^{-10} g cm^{-3}. The opacity without grains (*dashed curve*) drops to very low values at 1000 K. The opacity without molecules (*dotted curve*) does not display the opacity hump at 2000 K caused predominantly by water vapor and titanium oxide.

outer layers of red giant stars. Johnson and Whitaker (1975) and Whitaker (1976) have shown that ignoring molecules when computing the evolution of moderate mass stars can significantly alter calculations of their evolutionary tracks and properties.

The effects of varying the chemical composition are explored in Figures 4 and 5. Because of the way the grain condensation has been treated, calculations at other compositions must be restricted to temperatures above the regime of grains. Coarse mini-grids of Rosseland mean opacity were computed for temperatures between 1600 K and 5000 K for a range of different compositions. These results are presented in Table 3. They are presented for the purpose of making comparisons to the master grid. It should be remembered that they are interpolations based upon calculations in a (temperature, pressure) grid 3 times coarser than the master grid.

The standard composition of Cameron and Pine (1973) corresponds to abundances by mass fraction of $X = 0.71$, $Y = 0.27$, and $Z = 0.02$. The curve marked $Y = 0.2$ in Figure 4 has the same heavy element content but has had the helium mass fraction reduced to 0.20. It conforms closely to the values of the master grid, although differences as large as 0.5 dex do occur at some of the higher temperatures.

Also contained in Figure 4 are two curves for opacities with the abundance of the heavy elements decreased by factors of 10 and 100. As expected, the total opacity is diminished when the heavy element content is reduced. A very rough scaling law exists relating changes in the opacity to the overall abundance of heavy elements.

At low temperatures, which molecular species are present depends critically upon the ratio of carbon to oxygen. For $C/O < 1$, water vapor is the dominant molecular absorber at most temperatures; when $C/O > 1$, carbon-containing molecules such as CN and C_2 become the dominant absorbers. This changeover is caused by the great stability of the carbon monoxide molecule. Whichever element is least abundant is essentially completely locked up in CO, leaving the other element to form additional molecules which often are more effective absorbers than CO. These effects are illustrated in Figure 5. Altered C/O ratios are obtained by raising the abundance of carbon while keeping the abundance of all other elements fixed. As the C/O ratio is raised to 1, the opacity generally decreases as water vapor becomes less abundant. For C/O ratios greater than 1, the total opacity once again begins to rise as carbon-containing molecules become abundant.

This effect has serious implications for the study of the structure of the outer layers of M, S, and C stars

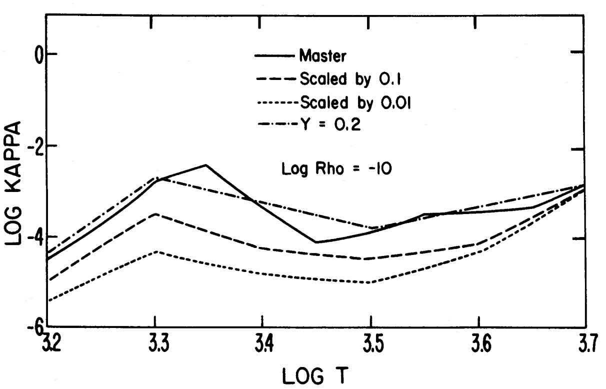

FIG. 4

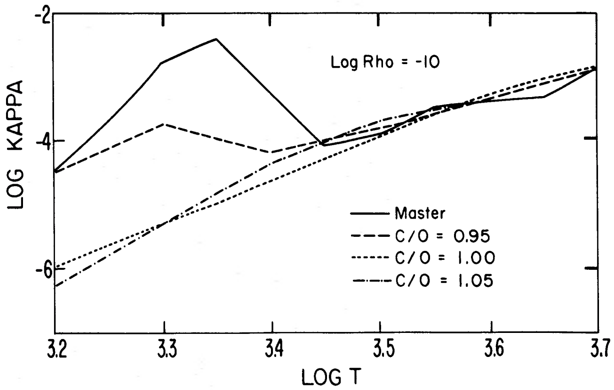

FIG. 5

FIG. 4.—The opacity with different compositions is illustrated at a constant density of 10^{-10} g cm^{-3}. The master grid assumes the chemical composition of Cameron and Pine (1973). The dot-dash curve has reduced helium but the same heavy element concentration. The dashed and dotted curves have heavy element concentrations scaled down from the master grid by 10 and 100 respectively.

FIG. 5.—The effect of variations in the C/O ratio is illustrated, again at a density of 10^{-10} g cm^{-3}. As the C/O ratio is raised toward 1, the abundance of several important molecular absorbers (particularly H_2O and TiO) diminishes and reduces the overall opacity. For C/O ratios greater than 1, new absorbers (CN, for example) become abundant and cause the opacity to begin to rise again from its minimum. More complex behavior is exhibited at other densities.

1983ApJ...272..773A

TABLE 3

MINI-GRIDS OF ROSSELAND MEAN OPACITIES (log κ)

	LOG ρ											
LOG T	-15.	-14.	-13.	-12.	-11.	-10.	-9.	-8.	-7.	-6.	-5.	-4.
					Metals Scaled by 0.1							
3.70					-2.945	-2.927	-2.587	-2.091	-1.569	-0.914	-0.333	0.162
3.60					-4.363	-4.136	-3.582	-2.810	-2.108	-1.505	-1.033	-0.643
3.50				-4.786	-4.731	-4.483	-4.026	-3.202	-2.549	-2.039	-1.706	-1.428
3.40			-5.270	-5.369	-4.985	-4.251	-3.274	-2.818	-2.623	-2.525	-2.446	
3.30		-5.610	-5.132	-4.534	-3.958	-3.508	-3.188	-2.961	-2.876			
3.20	-5.015	-4.995	-5.195	-5.419	-5.480	-5.007	-3.958	-1.695				
					Metals Scaled by 0.01							
3.70					-2.954	-2.941	-2.612	-2.150	-1.688	-1.186	-0.762	-0.417
3.60					-4.417	-4.363	-4.079	-3.485	-2.850	-2.194	-1.693	-1.287
3.50				-5.284	-5.232	-5.013	-4.619	-3.918	-3.335	-2.864	-2.494	
3.40			-5.663	-5.703	-5.386	-4.831	-4.140	-3.777	-3.578	-3.400	-3.240	
3.30		-6.030	-5.683	-5.243	-4.778	-4.343	-4.045	-3.847	-3.795			
3.20	-5.818	-5.865	-5.960	-6.026	-5.987	-5.444	-4.743					
					$\gamma = 0.20$							
3.70					-2.877	-2.796	-2.354	-1.655	-0.911	-0.167	0.413	0.851
3.60					-3.775	-3.317	-2.631	-1.955	-1.334	-0.752	-0.277	0.124
3.50				-4.070	-4.050	-3.794	-3.254	-2.262	-1.561	-1.066	-0.824	-0.636
3.40			-4.829	-4.900	-4.250	-3.230	-2.151	-1.722	-1.575	-1.525	-1.488	
3.30		-4.930	-4.336	-3.658	-3.081	-2.708	-2.355	-2.053	-1.891			
3.20	-4.154	-4.186	-4.492	-4.779	-4.796	-4.382	-3.503	-1.701				
					C/O = 0.95							
3.70					-2.914	-2.851	-2.416	-1.725	-0.983	-0.233	0.356	0.799
3.60					-3.800	-3.350	-2.662	-1.985	-1.390	-0.868	-0.386	0.040
3.50				-4.042	-3.995	-3.790	-3.407	-2.687	-2.078	-1.577	-1.183	-0.843
3.40			-4.765	-4.929	-4.707	-4.165	-3.339	-2.885	-2.627	-2.401	-2.197	
3.30		-5.334	-5.209	-4.657	-4.068	-3.735	-3.440	-3.183	-3.000	-2.840		
3.20	-4.913	-4.510	-4.627	-4.870	-4.871	-4.491	-3.743	-2.233				
					C/O = 1.00							
3.60					-3.648	-3.252	-2.706	-2.053	-1.388	-0.820	-0.350	0.036
3.40			-4.696	-4.904	-4.872	-4.609	-4.197	-3.735	-3.256	-2.834	-2.453	
3.20	-5.803	-5.976	-6.118	-6.226	-6.300	-5.954	-4.414	-2.833				
					C/O = 1.05							
3.70					-2.912	-2.848	-2.412	-1.721	-0.979	-0.228	0.361	0.805
3.60					-3.792	-3.340	-2.649	-1.962	-1.358	-0.830	-0.360	0.049
3.50				-4.027	-3.949	-3.675	-3.256	-2.669	-2.148	-1.698	-1.248	-0.844
3.40			-4.567	-4.653	-4.564	-4.325	-3.940	-3.601	-3.292	-2.859	-2.453	
3.30		-5.081	-5.108	-5.134	-5.186	-5.278	-5.168	-4.925	-4.413	-3.914		
3.20	-5.535	-5.707	-5.971	-6.219	-6.347	-6.246	-5.511	-3.053				

(Johnson 1982). Evolution studies which attempt to explain the transition from oxygen-rich to carbon-rich compositions will need to consider the changes in the total opacity as the C/O ratio changes. The maximum opacity effect of more than two orders of magnitude could produce important structural changes related, for example, to the efficiency of mixing.

IV. CONCLUSIONS

Rosseland mean opacity coefficients have been tabulated for a variety of compositions over the range from 700 K to 10,000 K. Effects of molecules and grains dominate at temperatures below 4000 K. It is expected that the inclusion of these opacity sources will have significant effects on the structure of cool stars and on the collapse of protostars and planets.

It has further been demonstrated that rather subtle changes in the chemical composition can result in dramatic changes in the opacity through alterations in the chemical equilibrium of molecules.

Several uncertainties remain in the present calculations. Although most molecular species have been treated by the accurate opacity sampling method, uncertainties in the spectral constants are still sometimes large. The inclusion of water vapor as a straight mean opacity also introduces a significant uncertainty for that important absorber. Similar uncertainties exist related to the physical properties of the grains, such as their shape and optical constants. It should further be emphasized that it has been assumed that the grains are in thermal equilibrium with the gas. In regions with rapidly varying thermal conditions, Fix (1969) has shown this to be a poor approximation.

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